

Indene

95-13-6 | DTXSID8042052

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 7.90 days

Global applicability domain: Inside

Local applicability domain index: 5.73e-01

Confidence level: 7.73e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Indan

Measured: 61.9

Predicted: 8.13

[Image not found](#)

Indene

Measured: 12.5

Predicted: 7.90

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Tetralin

Measured: 120

Predicted: 12.2

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Benzothiophene

Measured: 1650

Predicted: 21.4